J. Pure Appl. & Ind. Phys. Vol.2 (2), 126-131 (2012)

An Evaluation of Temperature Dependent Mean Energies of Excitation of Bose-Einstein Condensate

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(Received on : February 5, 2012)

ABSTRACT

Using the gapless second-order theory, the excitation energies and dynamics of the collective excitation for a partially condensed harmonic trapped quasi two dimensional bosonic gas has been studied. Our evaluated result for temperature dependent mean-energies show that the Kohn theorem is quite accurately satisfied for temperature $T<0.8\ T_c$.

Keywords: Collective, mode, Bose-Einstein Condensation, HFB-Popov approximation second order theory, Temperature dependent mean energy.

INTRODUCTION

The partially Bose-Einstein condensate trapped atomic gases provide an excellent test bench for developing finite temperature quantum theories. These weakly interacting systems can be modeled from first principles, and the experiments yield accurate and detailed information for comparison. Especially, the energies and decay rates of low-energy collective excitations have been measured tests for theoretical models.

For dilute condensates at temperature much lower than the condensate temperature T_c' the Bogoliubov approximation consisting of the Gross-Pitaevskii (GP) equation for the condensate wave function and the Bogoliubov equations for the quasi-particle excitations has proven to be accurate in describing the collective modes of the system. For higher temperatures one has to take into account the effects of the thermal gas component. Developing a theory that is computationally feasible and correctly models the system at temperature approaching T_c is a challenging task. The most commonly used finite-temperature theory is the Hartree-Fock-Bogoliubov-Popov (HFB-Popov) approximation. It neglects the dynamics of the thermal gas and the modifications in particle correlation induced by the condensate, but predicts quasi-particle energies in fair

agreement with the experiment. [1] The energy of the quadruple modes having azimuthal angular momentum quantum number $q_0=\pm 2$ deviates from the theoretical prediction for temperature above $0.6T_c$, but lately this deviation has been interpreted to mainly arise from improper modeling of the time dependent external potential used in the experiments to excite the collective modes.[2]
In order to take into account the leading order quasi-particle interactions and the correlation induced by the condensate in the inhomogeneous case, several theoretical approaches have been suggested.[3-10] The dynamics of the condensate and the thermal gas has also been studied using various kinetic theories.[11-15] The second-order theory for inhomogeneous, partially condensate gases presented in refs.[9,10] uses systematic perturbation theory to take into account the interaction terms in the Hamiltonian. Recently, this theory was extended to take into account the time-dependent external perturbation used to drive the system in the experiments, leading to an agreement with the measured energies and the damping rates of the collective modes.[2,16]

The second-order theories are computationally challenging, and there have been only a few numerical investigations of their prediction.[2,17,18] In this paper, we calculate the spectral distributions of the quasi-particle energies for a partially condensed Bose-Einstein Condensate (BEC) and compare the quasi-particle energies to the HFB-Popov results as function of temperature. Especially, we analyze the quasi-particle dynamics implied by the spectral distributions, observing that some collective modes should exhibit notable collapse and revival effects in trapped condensates. The possible existence of this phenomenon has been pointed out previously in Ref.[9,10], but it has not been studied in detail before. The collapse and revival of the excitations indicate that the energies and the damping rates alone do not suffice to describe the dynamics of these modes, i.e., the commonly used damped sinusoidal fit to the experimental data may be sufficient to describe the longer term dynamics of some modes.[19-24]

2.0 Mathematical formulae used in the evaluation

Second-Order Theory

In this section, one presents the second-order formalism for calculating the quasi-particle spectral distributions for a partially condensed, dilute, trapped BEC at finite temperatures. The starting point is the usual second-quantized Hamiltonian for structure less bosons

$$\hat{H} = \sum_{ij} \left\langle \hat{H}^{SP} \| J \right\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger + \frac{1}{2} \sum_{ij} \left\langle ij \left| V \right| km \right\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_m$$

Where the creation and annihilation operators for a particle in state |i) are denotes by â and respectively. The single particle Hamiltonian is given by the sum of the Kinetic energy and the external trapping potential as

$$\hat{H}^{SP} = -\frac{\hbar^2 \nabla^2}{2m} + V_{trap}(r)$$

and the dominant s-wave scattering at low temperature can be modeled by the effective low energy interaction potential

$$V(r) = \frac{4\pi a\hbar^2 \delta(r)}{m}$$

where a is the scattering length and m the atomic mass. This effective potential is inapplicable at high energies and leads to ultraviolet divergences in the theory which have to be renormalized in a proper way.

We choose to use canonical ensemble with fixed total number of particles N. By defining the bosonic number conserving operators

$$\hat{\alpha} = \left[\left(\hat{N}_0 + 1 \right)^{-1/2} \hat{a}_0 \right] \hat{a}_i \, ,$$

where the index 0 refers to the condensate state and $\hat{N}_0 = \hat{a}_0^\dagger \hat{a}_0$, one can write the Hamiltonian (1) as

$$\hat{H}_0 = \sum_{I=0}^{4} \hat{H}_i + 0\left(N_0 \left[\hat{\delta} / N_0 \right]^{5/2} \right)$$

Where,

$$\hat{H}_0 = N_0 \left[\left\langle \hat{H}^{SP} \| 0 \right\rangle + \frac{1}{2} N_0 \left\langle 0 \middle| V^S \middle| 0 \right\rangle \right]$$

$$\hat{H}_1 = \bar{N}_0 \sum_{i \neq 0} \left[i \left\langle \hat{H}^{SP} \| 0 \right\rangle + N_0 \left\langle i0 \middle| v^s \middle| 00 \right\rangle \hat{a}_i^\dagger + H.c. \right]$$

$$\hat{H}_2 = \sum_{ij \neq 0} \left[i \left\langle \hat{H}^{SP} \| j \right\rangle - \lambda \delta_{ij} + 2N_0 \left\langle 0i \middle| V^s \middle| j0 \right\rangle \hat{a}_i^\dagger \hat{a}_j \right]$$
$$+ \sum_{ij \neq 0} \left[\frac{N_0}{2} \left\langle ij \middle| V^s \middle| 00 \right\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger + H.c. \right] + \lambda \left(\hat{N}_{ex} \right)$$

$$\hat{H}_3 = \sum_{ijk \neq 0} \left[\sqrt{N_0} \left\langle ij \middle| V^S \middle| K0 \right\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger a_k + H.c. \right]$$

$$\hat{H}_4 = \sum_{ijkm \neq 0} \frac{1}{2} \left\langle ij \middle| V^s \middle| km \right\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_m$$

and $\hat{\delta} = \hat{N}_{ex} - \left\langle \hat{N}_{ex} \right\rangle$ is the number fluctuation operator of the non-condensate particles. The symmetries elements of the two-particle interaction potential V(r) are defined as

$$\left\langle ij \middle| V^s \middle| km \right\rangle = \frac{1}{2} \left[\left\langle ij \middle| V \middle| km \right\rangle + \left\langle ij \middle| V \middle| km \right\rangle \right]$$

and as

$$\lambda = \left\langle 0 \middle| \hat{H}^{sp} \middle| j \right\rangle + N_0 \left\langle 00 \middle| V^s \middle| 00 \right\rangle$$

Where the average number of atoms in the condensate state is given by $N_0 = N - \left\langle \hat{N}_{ex} \right\rangle$. Above the average {…} refer to quantum expectation values and H.c. for Hermitian conjugate.

In the zeroth-order approximation, one solves the ground state $\left| 0 \right\rangle$ of $\hat{H}_0$ alone, which makes the linear Hamiltonian $\hat{H}_1 1$ vanish. The excitations are found in lowest order by diagonalizing $\hat{H}_2$ and the number of the condensed particle N_0 has to be tuned such that the total number of particles satisfies $N = N_0 + N_{ex \cdot}$

It is convenient the use an orthonormal single-particle basis $\zeta_i(r) = \left\langle r \middle| i \right\rangle$ for all i = 0, 1…, where $\zeta_0(r)$ is the condensate wave function given by the Gross-Pitaevskii equation

$$-\frac{\hbar^2\nabla^2}{2m}\nabla^2\zeta_0(r)=V_{trap}(r)\zeta_0+N_0U_0\left|\zeta_0(r)\right|^2\zeta_2=\lambda\zeta_0(r)$$

with $U_0=4\pi a\hbar^2/m.$. The GP equation is obtained by minimizing $\langle\hat{H}_0\rangle$ with respect to $\zeta_0(r)$. Diagonalizing $\hat{H}_2$ using the Bogoliubov transformation

$$\begin{pmatrix} L(r) & M(r) \\ -M^*(r) & -L(r)\end{pmatrix}\begin{pmatrix} u_i(r) \\ v_i(r)\end{pmatrix}=\in_i\begin{pmatrix} u_i(r) \\ v_i(r)\end{pmatrix}$$

where

$$u_i(r)=\sum\nolimits_{j\neq 0}U_{ij}\zeta_j(r)$$

and

$$u_i(r)=\sum\nolimits_{j\neq 0}U_{ij}V_{ij}\zeta_j^*(r)$$

are the quasi particles. $\in_i$ the quasi-particle energies, and operator

$$L(r)=\hat{H}^{sp}-\lambda+2N_0U_0\left|\zeta_0^-(r)\right|^2$$

and $M(r)=N_0U_0\zeta_0^2(r)$ have been introduced. The quasi-particle amplitudes must satisfy the orthogonality and symmetry relations

$$\int dr\left[u_i(r)u_j^*(r)-\upsilon_i(r)\upsilon u_j^*(r)\right]=\delta_{ij}$$
$$\int dr\left[u_i(r)\upsilon_j(r)-\upsilon_i(r)\upsilon u_j(r)\right]=0$$

We express the particle operators in terms of the quasi-particle operators, yielding

$$p(r)=\sum_{i\neq 0}\left\{\left[\left|u_i(r)\right|^2+\left|\upsilon_i(r)\right|^2\right]n_i+\left|\upsilon_i(r)\right|^2\right\}$$

$$k(r)=\sum_{i\neq 0}u_i(r)\upsilon_i^*(r)(2n_i+1)$$

One finds the perturbative Hamiltonian

$$\hat{H}_{pert}=\Delta\hat{H}_0+\Delta\hat{H}_1+\Delta\hat{H}_2+\hat{H}_3+\hat{H}_4$$

Where the nonquadratic term $\hat{H}_3$ and $\hat{H}_4$ are to be calculated using the improved condensate wave function. Note that our notation $\Delta\hat{H}_i$ differs somewhat from that in Refs. 9 and 10.

The perturbation term $\Delta\hat{H}_0$ is just a real number and can be easily taken into account. In addition to it, in first-order perturbation theory only the terms $\Delta\hat{H}_2$ and $\hat{H}_4$ containing even numbers of quasi-particle operators contribute to the energy shift.

$$E_{pert}(s,1)=\left\langle s\left|\hat{H}_{pert}\right|s\right\rangle$$

where $|s\rangle$ is a quasi-particle occupation number eigenstate. In second-order perturbation theory, one can in fact neglect the terms $\Delta\hat{H}_2$ and $\hat{H}_4$ because it turns out that their contribution is of the same order as the contribution of the other terms in third-order perturbation theory.[9,10] Thus, one needs to calculate only

$$E_{pert}(s,2)\approx\sum_{r\neq s}\frac{\left|\left\langle r\left|\Delta\hat{H}_1+\hat{H}_3\right|S\right\rangle\right|^2}{E_s-E_r}$$

The quasi-particle energies are calculated as total energy changes in the system which the corresponding quasi-

particle occupation number by 1, while the total number of particles is held constant. This yields the corrected excitation energy

$$E_P(Z') = \epsilon_P + \Delta E_4^p + \Delta E_{shape}^p + \Delta E_\lambda^p + \Delta E_3^P(Z')$$

where the Δ terms are given in Eqs. and the complex energy parameter z′ should not be mixed with the fugacity. Calculating the excitation energies as function of z′ yields the dynamics of the excitations in the following way. The time evolution operator Û(t) of the system may be written in terms of the Fourier transform of the resolvent operator

$$\hat{G}(Z') = \left(Z' - \hat{H}\right)^{-1}$$

$$\hat{U}(t) = -\frac{\hbar}{\pi}\int_{-\infty}^{\infty} e^{-i\omega t}\,\mathrm{Im}\left[\hat{G}(\hbar\omega - i0)\right]d\omega$$

NUMERICAL METHODS

One considers a pancake-shaped system in a harmonic potential

$$V_{trap}(r) = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2 + \frac{1}{2}m\omega_z^2 z^2$$

where the trapping frequencies are $\omega_r = \omega_x = \omega_y$ and ω_z with $\omega_z >> \omega_r$. For sufficiently strong trapping potential in the z direction, the condensate wave function and the thermo-dynamically relevant quasi-particle amplitude can be approximated to be in cylindrical coordinates (r, θ, z) of the factorized form

$$\zeta_0(r) = \zeta_0(r)\sigma(z)e^{im\theta}$$

and

$$u(r) = u(r)\sigma(z)e^{i(q_\theta + m)\theta}$$

$$\upsilon(r) = \upsilon(r)\sigma(z)e^{i(-q\theta + m)^\theta}$$

where $\sigma(z)e^{-z^2/2(2a_z^2)}/\sqrt{a_z\pi^{1/2}}$ is a Gaussian profile and $a_i = \sqrt{\hbar/m\omega_i}$ are the harmonic oscillator lengths of the trap.

Table T_1

An Evaluated results of temperature dependent mean energies of the excitation modes using second order theory and also with HFB-Popov (Hartree-Fock-Bogoliubov) theory. The exact energy $\hbar\omega_r$ of the Kohn modes are also given

T/Tc	$E/\hbar\omega_r$		
	Second-order Theory	HFB-Popov Theory	Energy of Kohn Theory
0.0	2.058	2.153	1.079
0.1	2.092	2.224	1.082
0.2	2.145	2.278	1.097
0.3	2.181	2.324	1.116
0.4	2.226	2.359	1.132
0.5	2.274	2.396	1.138
0.6	2.345	2.438	1.142
0.7	2.378	2.473	1.145
0.8	2.455	2.524	1.154
0.9	2.481	2.545	1.166
1.0	2.550	2.607	1.178

DISCUSSION OF RESULTS

In this paper, we have evaluated the temperature dependent mean energies of excitation of Bose-Einstein Condensate. For numerical estimation, we have taken a model of pancake – shaped cloud consisting of N = 2000^{23} Na atoms trapped with trapping frequency ω_c = 25 x 350 Hz. The radial trapping frequency $\omega_r = \omega_x = \omega_y$ may be chosen freely with only the constraint $\omega_z > \omega_r$. The parameters are chosen from ref. 23. We have taken the theoretical formalism of M. Mottene, S. M. M. Virtaken and M. M.

Salomara.[25] In table T_1 , we have shown the evaluated results of temperature dependent mean energies of the excitation using second order theory together with HFB-Popov theory and exact energy of Kohn modes. Kohn modes are also called center of mass oscillation modes.[26] According to Kohn thorem[27] a system of harmonically trapped interacting particle in any eigenstate of the Hamiltonoian has an eigenstate with the amount $\hbar\omega_i$. The Bogoliubov theory, in which the thermal gas components is neglected, implies Kohn modes to have this exact energy. In higher order theories, the dynamics of the thermal gas and its interaction with the condensate have to be taken into account accurately obtained results in agreement with the Kohn theorem. In our calculation, it is shown that within the second order theory, the energy of the Kohn mode is very close to $\hbar\omega_r$ for temperature T < 0.8 Tc.

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